



Modelling and Numerical Simulation of a Passive Wall Incorporating a Phase Change Material

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ABSTRACT

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The energy consumption of a building is strongly dependent on the characteristics of its envelope. The thermal performance of external walls and roof represents a key factor to increase the energy efficiency of the construction sector and to reduce greenhouse gases emissions. Integration of Phase Change Material (PCM) in building envelope is undoubtedly one of the best ways to reduce the energy consumption due to decrease the energy requirement for maintaining thermal comfort by enhancing the thermal energy storage of the wall and the roof. This study deals with the numerical simulation of transient thermal behaviour of a plaster composite containing a microencapsulated phase change material (PCM) that can be embedded as a component in passive solar walls using a hybrid finite volume (FVM)/enthalpy method. First begins with the validation of our numerical model with the analytical results, we find that the results are identical, after using our model to study the thermal behaviour of the plaster /PCM composite wall. The results demonstrate in notable time shifting and reduction of the heat flux during the peak-hour time, due to PCM storage/release capacity during their melting/solidification, this good performance of thermal behaviour is associated with increased thickness of wall.

Keywords:

Phase change material; composite wall;

thermal behavior; finite volume;

enthalpy method

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1. Introduction

Energy consumption has significantly grown in the last decades, especially in the building sector, which has high contribution to the consumed large amount of conventional energy resources (fossil fuels) that drive environmental pollutions and climate changes. In addition, the dependency towards conventional energy resources will empties the sources more rapidly [1]. One of the solutions, which has attracted researchers and engineers, is to integrate phase change materials (PCM) into building

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envelopes or integrate in air conditioning system to improve buildings energy efficiency [2,3], consequently reducing dependency on fossil fuels and then contributing to a more efficient environmentally benign energy use [4]. Phase change materials (PCM) are characterized by storing and releasing a large amount of thermal energy during melting and solidification in narrow temperature ranges and decrease the temperature fluctuations, particularly in case of solar radiations loads [5]. PCMs have some disadvantages, such as the low heat-conductivity of the material. The thermal conductivities of PCM could be enhanced by using Nano-Graphite (NG)/ Graphene Nanoplatelets (GNP) [6,7].

The previously mentioned characteristics of PCMs (higher thermal energy storage) make it improve the thermal inertia of the building envelope [8], thermal inertia describes the sensitivity of materials to changes in temperature and therefore to reach equilibrium conditions (c' i.e., thermodynamic equilibrium) [9]. The role of the PCM is to increase the thermal capacity C which implies the increase in thermal inertia which globally plays the role of phase shifter and damper, i.e. it delays and reduces the effects amplitude of the climatic stress potential [10].

This property makes them ideal for passive heat storage in the envelopes of buildings. This tendency is confirmed by numerous papers available in the literature during the last 20 years. For a review, see in Ref [11]. The principle of the phase change material (PCM) use is simple. As the temperature increases, the material changes from solid to liquid phase. The reaction being endothermic, the PCM absorbs heat. Similarly, when the temperature decreases, the material changes from liquid to solid phase. The reaction being exothermic, the PCM desorbs heat [12].

Integrating Phase Change Materials (PCM) into building walls has been studied since the early 1980s, although their use has been increasing in the last decade, several research institutions around the world tested numerous configurations of gypsum boards, plasters, and concretes enhanced with phase-change materials (PCMs) [13].

Unfortunately, many reported durability problems, such as PCM that is leaking from the packages, or micro-containers, or surface sweating in case of the PCM-impregnated sheathing boards, have hampered earlier widespread adoption [14]. Therefore, in order to overcome these problems, a new technique of utilizing microencapsulated phase change material (MEPCM) in thermal energy storage system has been developed. The main merits of MEPCM over PCMs are as follows: (i) increasing heat transfer area; (ii) reducing PCMs reactivity towards the outside environment and controlling the changes in the storage material volume as phase change occurs. Since MEPCM was developed, it had been mainly used in the textile and building applications. It can increase the thermal mass of buildings and even clothing (i.e., increase their thermal energy storage capacity) without increasing their actual mass too much (i.e., without becomes a heavy) [15].

Nowadays, numerical modelling is mandatory to assess new buildings at the design stage. The building is a quite complex object going through to internal and external thermal influences. External influences are due to the local external weather. Internal influences come from solar radiative flux entering the building and internal loads.

In this context, it is important to develop a mathematical model to reproduce the thermal behavior and optimize the performance of the incorporation of the microencapsulated PCMs into different buildings elements. In this framework, Zalba *et al.*, [16] reviewed some theories and simulations of heat transfer within PCMs and highlighted the advantages of the enthalpy method to handle the energy equation in dealing with the PCM melting and solidification. Pierre Tittlein *et al.*, [17] used three different thermodynamical models for tested in order to simulate the unsteady thermal behavior of a cement mortar including phase change material. They concluded that the enthalpy method gives better results than the specific capacity method, then Younsi Zohir *et al.*, [18] they are used the numerical simulation of transient thermal behavior of a mortar wall containing a

microencapsulated phase change material (PCM) using a hybrid finite volume/enthalpy method. Such an approach was first validated by comparing their findings with experimental data from the literature. Simulation results indicated that the mortar wall embodying a PCM is capable to improve the storage of energy in the building materials and, thereby to contribute to the thermal comfort in the building. Finally, Mohamed Lachheb *et al.*, [19] study of the thermal behavior of new plaster composite containing a microencapsulated PCM by using numerical simulation, it is based on the enthalpy Method, they found that numerical findings match the experimental results.

On the other hand, there are other numerical studies more generalized in real weather conditions, their main goal is to understand the thermal behavior of PCM-enhanced building external walls throughout the year, to determine the parameters that lead to the improvement of the energy performance of these walls.

Among these studies, Mazzeo *et al.*, [20] they studied the dynamic thermal behavior of the external walls of buildings under conditions at the actual external and internal limits of operation., Pedersen [21] evaluated the effect of using PCMs in several positions within a wall configuration and presented some examples of the annual changes in energy performance caused by the integration of PCMs. The author has found that the implicit numerical solution is the most flexible method, a modified version of the enthalpy method is developed, in which the enthalpies of each node are updated with each iteration, then they are used to develop a specific heat equivalent C_p at each time step. Mazzeo *et al.*, [22] used a numerical simulation method for thermal dimensioning and for the evaluation of the energy behavior of the PCM layer contained in the exterior wall of the building. They defined a characteristic day for each month of a study and the numerical simulation was carried out by repeating this characteristic day for the whole month, which makes it possible to obtain indications on the behavior of the PCM throughout the year. This method was chosen because it could reduce the load of the digital simulation and make it possible to obtain the most suitable PCM thermophysical properties. Mazzeo and Oliveti [23] developed a model by used numerical solution based on the finite difference scheme, which gives a detail description of PCMs behavior with several bi-phase interfaces when subjected to non-sinusoidal boundary conditions.

This paper presents a numerical simulation of the transient heat transfer for study of the thermal behavior of new plaster composite containing a microencapsulated PCM that can be embedded as a component in building passive solar walls. A mathematical model based on the enthalpy method [24] has been developed and its related numerical solution using the finite volume method (FVM) was employed to investigate the temperature regulation effects resulting from the incorporation of microencapsulated paraffin in plaster matrix. First this model was validated by comparing the numerical simulation with analytical. Then, a parametric study was performed to study the effect of presence of PCM and the thickness of the composite wall (plaster PCM) on the reduction and the time shifting of the heat flux and temperature during the peak-hour time through such a composite.

2. Numerical Study

2.1 Mathematical Model

The numerical simulation of transient thermal behavior of a plaster wall containing a microencapsulated phase change material (PCM) using a hybrid finite volume/enthalpy method. Unlike explicit algorithms, the latent heat source term has been handled implicitly in the enthalpy equation. The current approach has been implemented considering a one-dimensional transient phase change problem with conduction.

The plaster may still be considered as a homogeneous medium. Therefore, to study the thermal behavior of this type of wallboard, we assume that this composite sample may be described via

average properties. To obtain a solution of the governing equations, several assumptions are key to understand limitations of the validity of the adopted approach. These are

- i. The heat transfer is one-dimensional and it is achieved via the thermal conduction
- ii. The mixture plaster/microencapsulated PCM is assumed to be homogeneous and isotropic [19] [25]
- iii. The thermo-physical properties (densities, heat capacities, and thermal conductivities) are constant although different in the solid and liquid phases. They are assumed to remain constant over time and independent of temperature (i.e., in the case where the MCPs change their state from solid to liquid or vice versa, depending on the increase or decrease in temperature, the values thermophysical properties of Plaster/microencapsulated PCM composites material also changes from state to state except the mass volume does not change, but the thermophysical properties are constant in each state) [26, 27]
- iv. Composite plaster microencapsulated PCM is supposed to have a melting point (isothermal phase change). Based on the above conjectures, the enthalpy formulation for the conduction-controlled phase change can be written as [28]

$$\frac{\partial H}{\partial t} = \nabla(k\nabla T) \quad (1)$$

where k , T and H represent respectively the thermal conductivity, the temperature, and the total volume enthalpy.

By working in an isothermal, unidimensional linear domain of length D , and assuming that the hypotheses mentioned above are valid, the energy balance based on the enthalpy method in a Cartesian framework is expressed as Eq. (1). The total volume enthalpy can be broken down into two parts, a sensitive part and another latent one given by

$$H = h + \rho f L \quad (2)$$

With f , ρ , L , and h indicate the volume fraction of the liquid, the density, the latent heat and the sensible enthalpy of the PCM. The latter can be expressed as a function of the temperature and the specific thermal capacity by the following relation

$$h = \int_{T_m}^T \rho c dT \quad (3)$$

where T_m denotes the melting temperature of the PCM. In the case of an isothermal phase change, the liquid phase fraction f is defined as

$$f = \begin{cases} 0 & \text{if } T > T_m \\ 1 & \text{if } T < T_m \end{cases} \quad (4)$$

A general enthalpy formulation can be given by the non-linear relation with taking into account the sensitive and latent parts

$$\frac{\partial h}{\partial t} = \nabla(\alpha \nabla h) - \rho L \frac{\partial f}{\partial t} \quad (5)$$

where, $\alpha = \frac{k}{\rho c}$ is the thermal diffusivity. The previous equation can be written in terms of temperature in the following form

$$\rho c \frac{\partial T}{\partial t} = \nabla(k \nabla T) - \rho L \frac{\partial f}{\partial t} \quad (6)$$

The above equation along with initial/boundary conditions and Eq. (3)-(4) represents the mathematical model governing the isothermal phase change problem with conduction. It is worth noting that such a formulation is suitable, since the liquid fraction is regarded as a source term. Since the Eq. (5) is non-linear, it can only be solved numerically. By examining these last Eq. (5) and (6) along with initial/boundary conditions and Eq. (3)-(4) represents the mathematical model governing the isothermal phase change problem with conduction. It is worth noting that such a formulation is suitable, since the liquid fraction is regarded as a source term, we note a non-linearity of the problem. The relationship between temperature and the difference in total enthalpy prevents resolution in the form of a classical linear equation system. The problems of this form it can only be solved numerically by iterative methods.

2.2 Discretization of The Mathematical Model

Using the finite difference method, with an implicit scheme, Eq. (6) approximates such that

$$T_i^{n+1} = \frac{\alpha \Delta t}{(\Delta x)^2} (T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}) + T_i^n - \frac{L}{c} (f_i^{n+1(k)} - f_i^n) \quad (7)$$

These equations can be written algebraically. For example, Eq. (7) is expressed algebraically as follows

$$a_p T_i^{n+1} = a_E T_{i+1}^{n+1} + a_W T_{i-1}^{n+1} + T_i^n - \frac{L}{c} (f_i^{n+1(k)} - f_i^n) \quad (8)$$

with

$$a_p = 1 + a_E + a_W \text{ and } a_W = a_E = \alpha \frac{\Delta t}{\Delta x^2}$$

where f is the K eme evaluation of the liquid fraction at node i .

The equation obtained (8) is a nonlinear equation, this imposes an iterative resolution. The algorithm for solving a tri-diagonal matrix equation system used to solve this system of equations is called TRIDAG (Tri-Diagonal Matrix Algorithm), also known as the Thomas algorithm or TDMA. This solver is really a formula for recursive use in order to solve this matrix equation using Gauss elimination. When the coordinate point x_i is changing phase, the temperature is equal to T_m this leads to a difference in sensitive enthalpy h_i zero.

At iteration $K + 1$

$$a_p T_m = a_E T_{i+1}^{n+1} + a_W T_{i-1}^{n+1} + T_i^n - \frac{L}{c} (f_i^{n+1(k+1)} - f_i^n) \quad (9)$$

In order to obtain the correction of the liquid fraction necessary to advance the phase change front, we subtract Eq. (8) and Eq. (9)

$$f_i^{n+1(k+1)} = f_i^{n+1(k)} + \omega a_p \frac{c}{L} (T_i^{n+1} - T_m) \quad (10)$$

where ω is a relaxation coefficient, its role is to reduce the oscillations and avoid divergence.

In practice, this update (10) of the liquid fraction is applied in each of the control volumes of the calculation domain after the k th solution of the energy conservation equation. For control volumes which do not change or which have finished their phase change, the liquid fraction is preserved using a second correction

$$f_i = \begin{cases} 0 & \text{if } f_i^{n+1(k+1)} < 0 \\ 1 & \text{if } f_i^{n+1(k+1)} > 1 \end{cases} \quad (11)$$

This second correction is valid for all the points having a liquid fraction outside the interval $[0,1]$. The two corrections are used, after solving the system of equations, in order to establish the new value of the liquid fraction. This operation is repeated until the convergence satisfaction.

3. Numerical Validation

In this part, 1D numerical results are compared with results obtained from the analytical solution of a Dirichlet type problem. The analytical solution refers to a problem on a half-line of infinite length [29], the numerical solution is calculated on a finite domain. One chose a sufficiently large field of computation to avoid that the temperature on the right border does not undergo too pronounced changes at the time of the resolution. The properties used are those characterizing water.

3.1 Ice Melting

This test concerns the melting of ice whose thermophysical properties (solid, liquid) which are given in Table 1. Initially, the ice at a uniform temperature of $T_0 = 268.15$ K. Suddenly the temperature on the left side of the domain is raised to $T_w = 293.15$ K and the melting of the ice begins at $x = 0$. The temperature of the right border remains constant at $T = 268.15$ K. The boundary conditions of this example are as follows

$$\begin{array}{ll} \text{at } t = 0 ; 0 \leq x \leq L & T = T_0 < T_m \\ \text{at } x = 0 ; t > 0 & T = T_w > T_m \\ \text{at } x = L ; t > 0 & T = T_0 \end{array}$$

where L is the thickness.

Figure 1 and 2 show the history of the displacement of the interface of the ice melting and the profile of the Temperature at the final time according to the abscissa x respectively. It is found that our numerical findings match the analytical results. This indicates that our numerical model is suitable for the treatment of such cases.

Table 1
 Physical properties for water and ice [30]

Variable	Ice	Water
k (W/m.K)	1.92	0.606
C_p (J/kg.K)	1960	4181
ρ (kg/m ³)	917	1000
L (kJ/kg)	333.40	
L (m)	1.00	
T_o (K)	268.15	
T_m (K)	273.15	
T_w (K)	293.15	

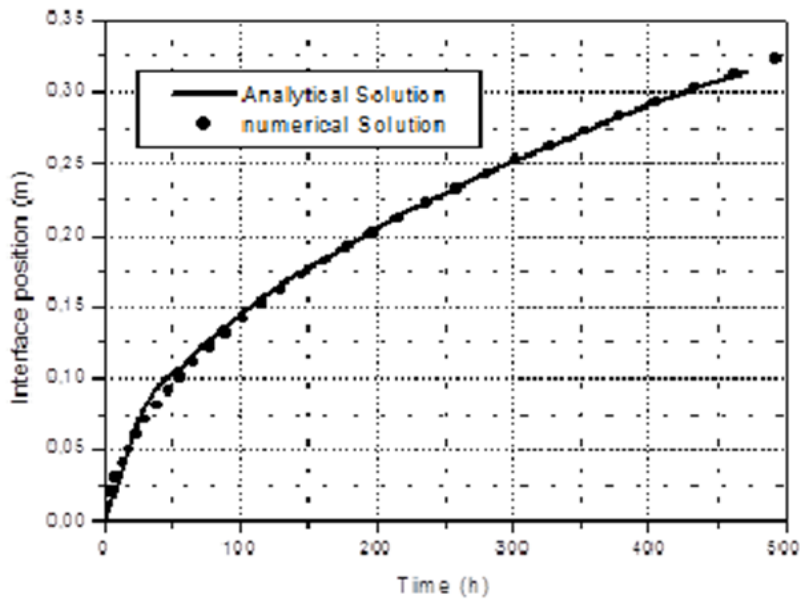


Fig. 1. History of the displacement of the interface for ice melting

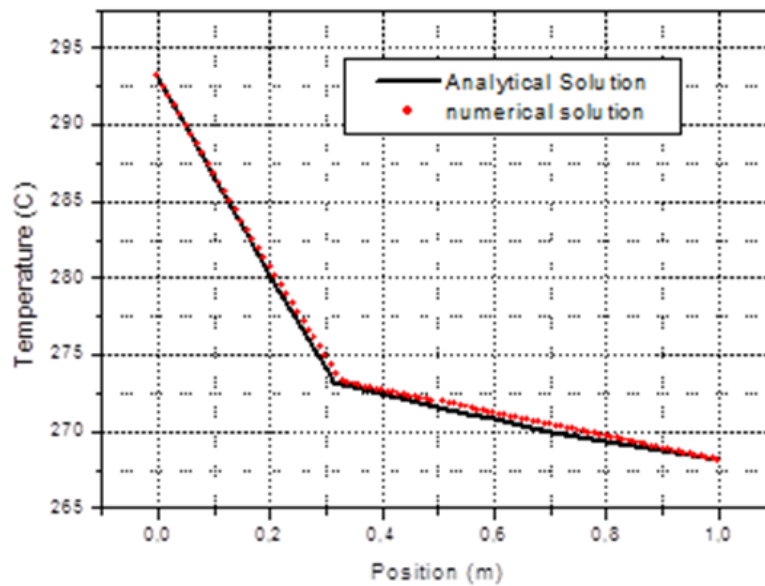


Fig. 2. Temperature profile at end time for test 1 $t=17e+5s$

4. Thermal Characteristics of Plasterboard / PCM with Sinusoidal Outside Temperature Variation

In this section, a numerical study was carried out to study the influence of the plaster-microencapsulated PCM composite on the temperature control of the building. The PCM chosen having a melting temperature ($T_m = 26^\circ\text{C}$), to carry out this study. All the properties of the materials constituting this solar wall are indicated in Table 2.

Table 2

Thermophysical properties of materials (Plaster MEPCM) used in construction walls [19]

Material	Plaster	Plaster-PCM 90/10
Solid state thermal conductivity (W/m.K)	0.301	0.299
Liquid state thermal conductivity (W/m.K)	-	0.236
Solid state thermal capacity (J/kg.K)	835	915
Liquid state thermal capacity (J/kg.K)	-	725
Latent heat (J/kg)	-	11265
Density (kg/m ³)	1292	1213

The solar wall of thickness Lx , is initially at a temperature $T_0 = 20^\circ\text{C}$ ($T_0 < T_m$). At $t > 0$, we imposed a sinusoidal variation of the outside temperature. This condition represents the daily variation in the temperature of the atmosphere. The imposed boundary conditions were created using historical climatic data sets. The boundary conditions are schematized in the following Figure 3 and are also presented the following

- i. Outdoor temperature: $T_{a,ext} = 24 + 8 \sin(\omega.t)$
- ii. Indoor temperature: $T_{a,int} = 23^\circ\text{C}$
- iii. The external convection coefficient between the external surface of the composite wall and the atmosphere: $h_{ext} = h_1 = 18 \text{ W/m}^2.\text{K}$
- iv. The internal convection coefficient between the internal surface of the composite wall and the ambient atmosphere of the room: $h_{int} = h_2 = 9 \text{ W/m}^2.\text{K}$

where t is the time (s) and $\omega = 2\pi/\tau$, τ being the period (24 h).

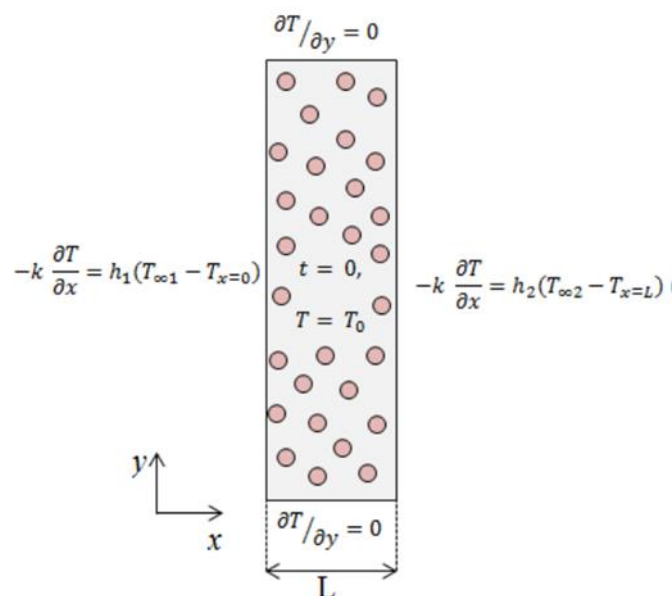


Fig. 3. Computational domain with boundary conditions

4.1 Results and Discussions

4.1.1 Effect of the presence of PCM

In this step, we have treated the numerical results obtained for thermal study of wallboard composite plaster- microencapsulated PCM solar wall with percentage of 10% by weight of PCM, a layer of wall thickness ($e = 12\text{cm}$), The purpose of this calculation is to determine the thermal behavior of a wall solar containing microencapsulated PCM for a study period of two days (48 h).

Figure 4 shows the comparison between the inner and outer surface temperature profiles in with and without PCM, in this case, we note that the amplitude of temperature oscillation in outside face is very high compared to that of inside face of the wall in the both cases.

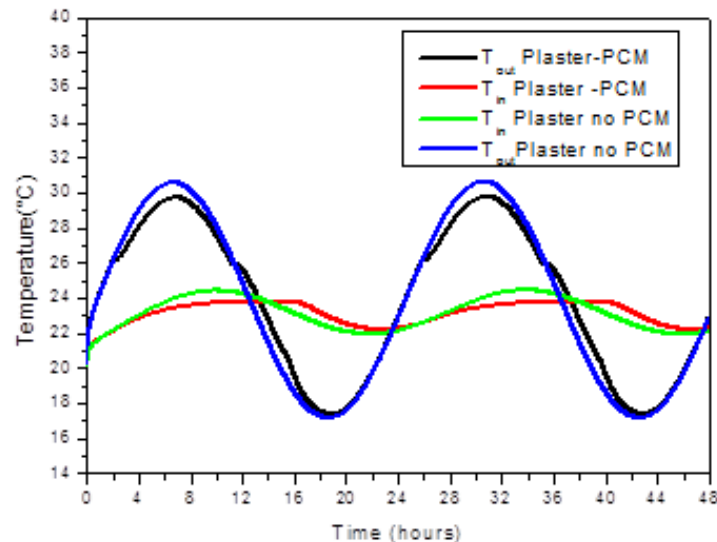


Fig. 4. Comparison between the inner and outer surface temperature profiles, with and without PCM under periodic thermal excitation of wallboard Plaster/microencapsulated PCM composites (90/10)

In this study, we will focus on the effect of the presence of PCM on the thermal behaviour of the wall, on this, we note in the case without PCM the inner face the amplitude of temperature is high compared to in the case with PCM, the inner surface temperature without PCM reaches a maximum $T_{w,in-no\ PCM} = 24.52\text{ }^\circ\text{C}$ whereas the inner surface temperature with PCM reaches a maximum $T_{w,in-PCM} = 23.72\text{ }^\circ\text{C}$, and a shift of about 6.67 h in the peak-hour load was observed and the existence of a plateau on the curve of $T_{w,in-PCM}$, This can be explained by the increase of the thermal inertia of the walls due to the charge and discharge processes during the 24-h time period of PCM. However, the charging and discharging process is not fully present throughout the thickness of the wall, only layers located on the outside of the wall were involved in the phase change process, this is due to the insufficient heating and cooling time for the charging and discharging process to take place throughout the wall, this explains that the inner surface temperature of the wall $T_{w,in-PCM}$ is lower than the melting temperature T_m , this is due to the large thickness of the wallboard, the choice of the thickness of $e = 12\text{ cm}$ is not practical in the building construction, and this thickness makes the wallboard too heavy. So, to allow all or most PCMs to load and unload through the thickness of the wall we need to decrease the thickness of the wallboard, in this case we also get a light wallboard which is more practical in building construction with increased thermal mass due to the presence of PCMs. In the next section we study the thermal behavior of a wallboard Plaster/microencapsulated

PCM composite as a function of thickness to see which optimum thickness gives a reduction in energy consumption and thermal comfort inside the home.

4.1.2 Effect of the variation in the thickness

The variation of the thickness of the Plaster/microencapsulated PCM is also a key parameter which can influence the thermal efficiency of the building, we integrate 10% of the PCM by weight to see the temporal variation of the temperature and the flux of the interior surface of the wall. For this, three different thicknesses 1 cm, 2 cm and 3 cm were considered.

The Figure 5 and 6 present a comparison of the heat fluxes and temperature variation respectively of the wallboard interior face for three thicknesses, we appreciated that the simulated temperature variation and heat fluxes of the wallboard has the same behavior for the different thickness values.

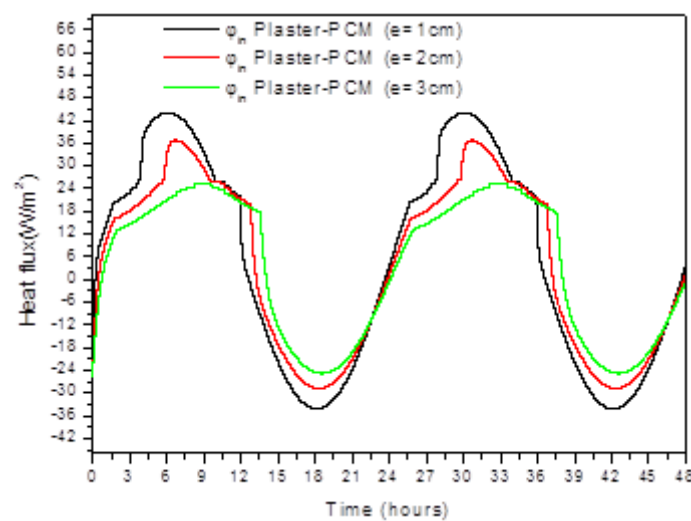


Fig. 5. Inner surface heat flux variation for different thickness of the wallboard Plaster/microencapsulated PCM composite (90/10)

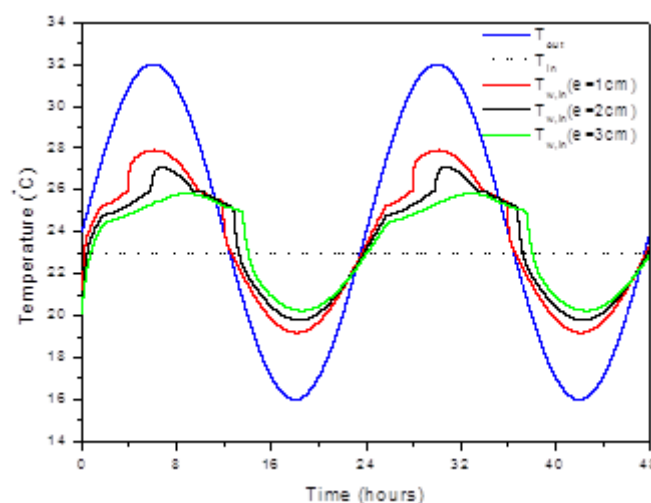


Fig. 6. Temporal variation of the temperature of the internal face for different thicknesses of the wallboard plaster/ microencapsulated PCM (90/10)

On the other hand, the oscillations amplitude of the heat flux and the temperature, is dependent on the variation of the thickness and are decreased with the increase in the thickness. For the case where the thickness of the layer is 1 cm, the thermal flux of the internal surface reaches a maximum of 43.98 W / m^2 , while for the case where the thickness of the layer is 3 cm, the flux reaches a maximum of 25.41 W / m^2 . This shows that the increase in thickness leads to having a wall defined by its great thermal inertia.

And for the temperature in the case where the thickness of the layer is 1 cm, the temperature of the internal surface reaches a maximum of $27.94 \text{ }^\circ\text{C}$, while in the case where the thickness of the layer of the wallboard is 3 cm, the temperature reaches a maximum of $25.88 \text{ }^\circ\text{C}$. That is, an estimated difference $2.06 \text{ }^\circ\text{C}$ between the two thickness cases. This can be explained by the fact that when the thickness is increased, the thermal inertia of the wall increases, the amplitude of the oscillations of the internal temperature is reduced and becomes more stable. The observed oscillation also presents a significant phase shift with the oscillation of the outside temperature. Based on these results, it may be stated that the thermal comfort of a building can be improved by increasing the wall thickness, but this increase in the thickness of the wall has a limit.

You must choose the thickness that brings us reduction of consumption energy and occupant comfort. In addition, the energy performance of this composite wall depends on other parameters related to the characteristics of PCM among which, the melting temperature of PCM which should be as close as possible to the set temperature of the room [31], the heat latent phase change which must be higher [32], little or no super cooling, low vapor pressure, good thermal and chemical stability and self-nucleation behavior [33], high thermal conductivity in liquid and solid phase (but not always), low density variation, high density, compatibility with container materials, nontoxic, non-flammable, non-polluting, cheap and abundant [34].

5. Conclusion

In the present work, the thermal performance of the new plaster incorporating the microencapsulated PCM, which can be used as a wall element for the temperature control of buildings, has been studied numerically. For this reason, a numerical model, based on a finite volume/enthalpy method, has been implemented. This approach was first validated by comparing our results with the analytical results we find that the results are identical. Then, a parametric study was carried out using the developed model, in order to study the effect of PCM on the temperature regulation of the building. The following conclusions can be drawn from our main results

- i. The enthalpy model based on the hypothesis of a binary mixture has been successfully validated by analytical data.
- ii. The increased thickness of the plaster/PCM wallboard improves the thermal comfort of the building, but a certain critical value must not be exceeded, which determines, depending on the requirements, the reduction of energy consumption and occupant comfort.

In summary, our results show that the effectiveness of the new composite material is remarkable. The incorporation of such a composite material in a building envelope improves thermal comfort, and reduce energy consumption in buildings.

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